Loss Function of Complex Oxides: The Case of CrO_2

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Transition-metal oxides represent important realizations of strongly-correlated materials, featuring some of the complex electronic processes which are thought to be relevant in the cuprate high-temperature superconductors. *On the basis of a newly-developed response code based on time-dependent density-functional theory, we have uncovered novel collective electronic phenomena*. The sharp excitation featured in Figs. 1 and 2 owes its existence to a subtle interplay between localized *d*-orbitals and the crystal environment in rutile CrO_2. This mode impacts the screening properties at the Fermi surface. Similar studies for other strongly-correlated materials are underway.

Oscar Restrepo (graduate student supported by this grant) and A. G. Eguiluz, to be submitted to Physical Review Letters.

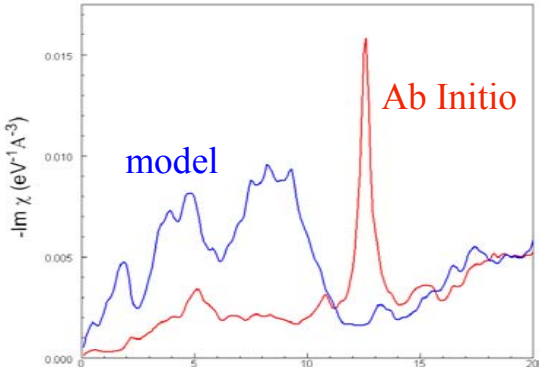

Fig. 1. Loss Function of CrO_2, calculated for q=2.5 Å^{-1}. A novel, sharp collective mode is not realized in a "model" calculation which ignores the "crystal local fields."

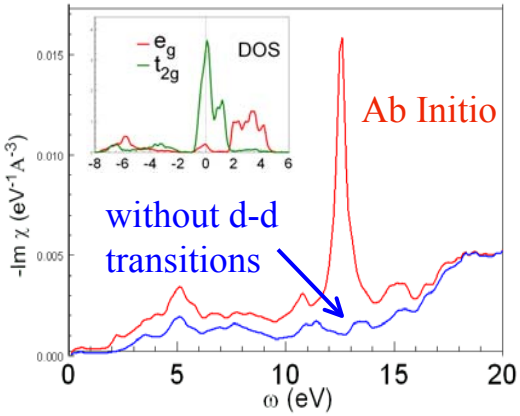

Fig. 2. If electron-hole excitations involving e_g states (see inset) are ignored, the collective mode is destroyed.